

Diphenylamine  
122-39-4 | DTXSID4021975

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.10e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.81e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Fenitrothion</div> <div>Measured: 6.70e-04</div> <div>Predicted: 9.49e-06</div>	<div>Image not found</div> <div>Benzyl cinnamate</div> <div>Measured: 7.91e-04</div> <div>Predicted: 1.93e-05</div>	<div>Image not found</div> <div>Benzene, pentamethyl-</div> <div>Measured: 9.08e-07</div> <div>Predicted: 3.16e-01</div>
<div>Image not found</div> <div>2-Phenylphenol</div> <div>Measured: 2.73e-05</div> <div>Predicted: 2.57e-04</div>		